Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Molecular Dynamics study of tetracosane monolayers adsorbed on graphite[1] L. FIRLEJ, B. KUCHTA, M.W. ROTH, University of Northern Iowa, Department of Physics, PAUL A. GRAY, University of Northern Iowa, Department of Computer Science, CARLOS WEXLER, University of Missouri Columbia, Department of Physics and Astronomy — We present the results of Molecular Dynamics (MD) simulations of tetracosane ($C_{24}H_{50}$) monolayers physisorbed on graphite. $C_{24}H_{50}$ molecules have explicit hydrogens and the graphite is represented by six graphene layers. We focus our analysis on the microscopic mechanism of melting, experimentally observed at $T = 340$ K. We are looking for the pre-melting transformations with emphasis on the correlation between translational disordering of molecules and their internal degrees of freedom. We analyze several order parameters and their fluctuations along the MD trajectories. We show that the all atom representation of $C_{24}H_{50}$ is much more sensitive to the model of intramolecular interactions than united atom model. Footprint reduction during melting involves a simultaneous loss of intramolecular and translational order.

[1]Acknowledgment is made to the Donors of the American Chemical Society Petroleum Research Fund (PRF43277 - B5), the University of Missouri Research Board, and the D.O.E (DE-FG02-07ER46411).

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Date submitted: 14 Dec 2007 Electronic form version 1.4